

K. Braun-Munzinger,\* J. A. Dunningham, and K. Burnett  
*Clarendon Laboratory, Department of Physics, University of Oxford,  
Parks Road, Oxford OX1 3PU, United Kingdom.*

In this paper we examine the excitations observable in atoms confined in an optical lattice around the superfluid-insulator transition. We use increases in the number variance of atoms, subsequent to tilting the lattice as the primary diagnostic of excitations in the lattice. We show that this locally determined quantity should be a robust indicator of coherence changes in the atoms observed in recent experiments. This was found to hold for commensurate or non-commensurate fillings of the lattice, implying our results will hold for a wide range of physical cases. Our results are in good agreement with the quantitative factors of recent experiments. We do, however, find extra features in the excitation spectra. The variation of the spectra with the duration of the perturbation also turns out to be an interesting diagnostic of atom dynamics.

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## I. INTRODUCTION

Interest in the properties of atomic BECs in optical lattices, both theoretical [1, 2, 3] and experimental [4, 5, 6, 7] is growing rapidly at the moment. This is due partly to the possibility of studying the physics of a strongly correlated atomic system for a wide range of the relevant parameters. In particular, the observation of the superfluid (SF) to Mott insulator (MI) transition has caused a great deal of excitement in future possibilities for the field. Atomic arrays in optical lattices also promise a potentially significant route to quantum information processing [8].

The recently introduced experimental technique of adding a linear potential gradient to the lattice has opened up a new way to study the phase transition from SF to MI. By carrying out numerical simulations of this technique we are able to compare the effect of this tilting on states with various degrees of reduced number fluctuations, i.e. number squeezing. Our focus is on the highly squeezed regime in the region of the phase transition.

We will first give a brief overview of the Bose-Hubbard model and the numerical method we use to simulate the evolution of the trapped condensates in the presence of the applied field. We then present results of simulations for a range of initial states, lattice sites and occupation numbers. In our discussion, we focus on the time dependence of excitations and the effect of non-commensurate filling. We find that the variance of the number of atoms at each site is a robust indicator of coherence changes, even in non-ideal systems (i.e. finite and non-commensurate). Our results are in excellent qualitative agreement with recent experiments [7].

## II. BOSE-HUBBARD MODEL AND THE ENERGY GAP

The system we simulate in this paper consists of a BEC trapped in a one-dimensional lattice. We believe, however, that our results have fairly broad implications for three dimensions as the phenomena we see are of a generic nature. The behaviour of this system is described by the Bose-Hubbard-Model (BHM) [9, 10], i.e.

$$H = \sum_j E_j \hat{n}_j + \frac{1}{2} U \sum_j \hat{n}_j (\hat{n}_j - 1) - J \sum_{\langle j, k \rangle} \hat{a}_j^\dagger \hat{a}_k. \quad (1)$$

Here  $\hat{a}_j, \hat{a}_j^\dagger$  stand for the bosonic annihilation and creation operators,  $\langle j, k \rangle$  denotes summation over nearest neighbours,  $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$  is the bosonic number operator, and  $E_j$  the energy offset of each site.  $J$  is the hopping matrix element between sites and  $U$  the (repulsive) interaction constant for bosons sharing a site. For numerical simplicity, we will consider modest-sized lattices with between four and eight sites and average occupation numbers of up to three atoms per site, i.e.  $n_{\text{av.occ.}} = 1, 2, 3$ . Experiments that demonstrate the MI transition involve many more lattice sites than this [4, 5, 6, 7]. However, by considering the evolution of locally determined quantities we should be able to

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\*Electronic address: k.braun-munzinger1@physics.ox.ac.uk

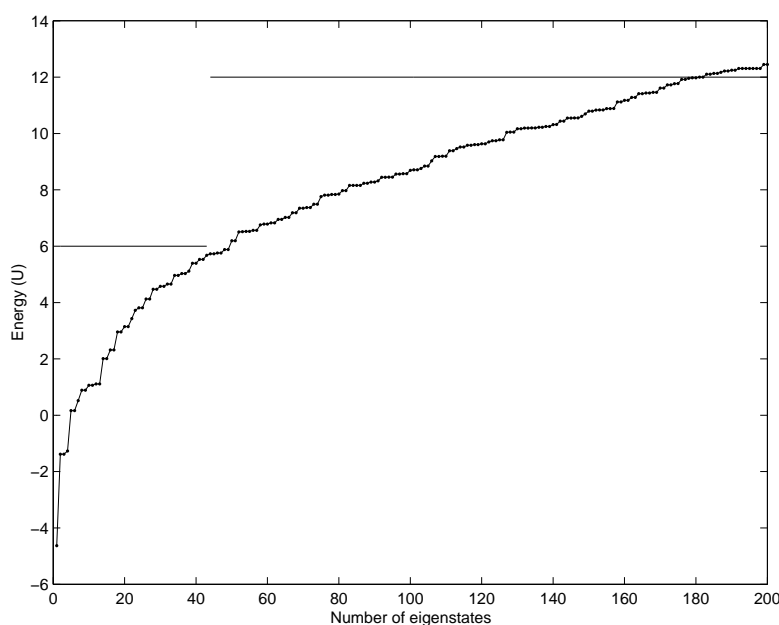


FIG. 1: This shows the first 200 eigenstates for  $U=6$  and  $J=1$  (dots) and  $U=6$  and  $J=0.0001$  (thin line)

gain some insight into the behaviour of larger lattices. We will see that this is a reasonable assumption from the fact that the results for different numbers of lattice sites show similar excitation patterns. We study our system by solving the coupled equations of motion in the number state basis using an embedded fifth order Runge-Kutta approximation [11]. The initial states for the simulations are the eigenstates of (1) for different values of  $U/J$ . The squeezed states are then probed by ‘tilting’ the chain of sites. In our simulations, this potential gradient is implemented by adding an onsite energy  $E_j$  to each site’s ground state energy. The change in the number variance  $V$  is then studied after the potential gradient has been applied for a fixed length of time  $\tau_{\text{perturb}}$  with instantaneous turn on and turn off. We calculate the number variance  $V$  as

$$V = \langle (\hat{n}_i)^2 \rangle - \langle \hat{n}_i \rangle^2 \quad (2)$$

where  $\hat{n}_i$  is the number operator for site  $i$  and  $\langle \rangle$  denotes the ensemble average. We have chosen to use  $V$  as our measure, because it has the great advantage of being a locally determined quantity, making it less sensitive to the finite size of the lattices [12]. This means that a study of  $V$  for modest lattice sizes should allow us to make predictions that are consistent with larger lattices. In the experiment [4], excitations were measured via changes in the interference patterns observed in the distribution of atoms released from the lattice. The excitations, caused by tilting the lattice, manifest themselves in an increased width of the main interference peaks [4] observed when the system is taken back into the SF phase. In our simulations, the effect of the applied tilt was much clearer in the local variable  $V$ . For further discussion of the use of number variance in the theory of BEC and of the relationship between those observables see [10, 12, 13, 14]. We should note that the number variance may be measured experimentally by studying the collapse and revival times of the relative phase between sites. The relationship is given by [15, 16]:

$$\tau_{\text{collapse}} \approx \tau_{\text{revival}} / \sqrt{V}$$

One of the main indicators of the MI state is an energy gap. When present it implies that atoms can only move between sites if they possess sufficient energy. When tilting a lattice, one changes the relative potential energy of the sites and hence the energy available for a hop. Accordingly, if the energy difference between sites is comparable to the energy gap, boson hopping should occur. In fact, we expect this to be a resonant process when the energy variation between sites produced by the applied field matches the energy gap. Such resonant behaviour - which is termed a particle-hole excitation - is observed both in the experiments [5, 7] and the simulations we present. In the SF phase there is no gap in the excitations and a flow of atoms will occur at all values of the tilt. For an infinite one-dimensional lattice, mean field and quantum Monte Carlo calculations indicate that the phase transition is located at  $U/J \approx 5.8$  [2, 17, 18]. In a finite size lattice, the phase transition is not sharp and neither is the onset of a gap. In fact, a plot of the eigenstates close to the phase transition ( $U/J = 6$ ) shows a multitude of possible transitions (see Fig. 1 and 2). Obviously, the simple Mott insulator picture with an energy gap of  $\approx U$  will not explain all excitations possible

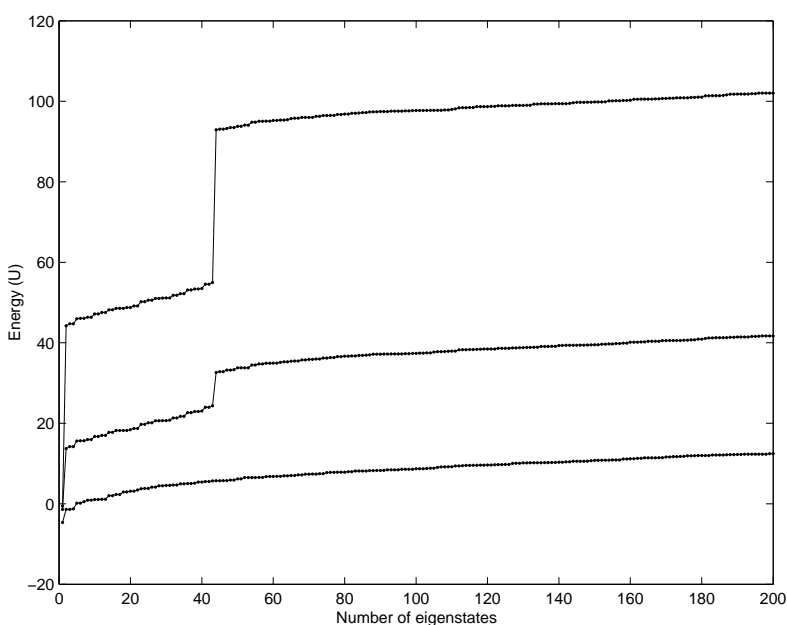


FIG. 2: This shows the first 200 eigenstates for  $U = 6, 20$ , and  $50$  and  $J = 1$ .

for this range of eigenstates. Indeed, we observe a broad smooth curve superimposed on Mott insulator peaks that slowly vanishes with increased  $U/J$  (see Fig. 6). Recent experimental results for lattices with about 100 sites show very similar features [7]. Fig. 2 shows examples of the eigenstate spectrum for the range of initial states studied in this paper. Close to the phase transition ( $U/J = 6$ ), no gap is observable. In contrast, states further into the Mott regime ( $U/J = 20$  and  $U/J = 50$ ) show a definite gap, even though the first and second bands are still broadened.

In the next section, we will present our results before the background of the theory just discussed.

### III. RESULTS

We prepare states with different degrees of relative number squeezing and then apply a tilt for a perturbation time  $\tau_{\text{perturb}}$ . We then recalculate  $V$  from the resulting wave function. This enables us to determine the effect of a fixed tilt on an initial state as a function of the initial squeezing, the average occupation  $n_{\text{av.occ.}}$  and  $\tau_{\text{perturb}}$ . In other words, we can study the dependence of excitations on the perturbation time as well as on the occupation number. The results of simulations to that effect can be seen in Fig. 3-7 where  $V$  is plotted as a function of the applied tilting potential for various initial states and durations of tilting. For a perfectly squeezed state in an infinite lattice, we would expect resonances at integer multiples and integer fractions of the interaction energy  $U$  (i.e., at  $U \cdot n_1$  and  $U/n_2$ ,  $n_1, n_2$  being integers,  $0 < n_1 \leq \text{total number of atoms}$  and  $0 < n_2 < \text{number of sites}$ ). It is reasonable to suppose that a resonance at  $U \cdot n_1$  corresponds to  $n_1$  particle-hole pairs being created in adjacent sites while a resonance at  $U/n_2$  corresponds to the creation of a particle-hole excitation in two sites  $n_2$  sites apart (i.e. in site  $i$  and site  $i + n_2$ ).

Even for a modestly sized lattice (in this case four lattice sites) the location of peaks was in good agreement with the theoretical predictions for an infinite lattice. This is clear in Fig. 3, which shows excitations for filling factors of one, two and three respectively.

All the plots show one-particle excitations at  $E_{\text{tilt}} \approx 1 \cdot U$  and  $E_{\text{tilt}} \approx 0.5 \cdot U$ . For  $n_{\text{av.occ.}} \leq 2$ , two, three and even four-particle excitations appear. Most likely due to the superposition of a broad continuous spectrum with discrete peaks, there is a slight shift ( $\approx 0.1 - 0.2 \cdot U$ ) of the maximum of the resonance at  $E_{\text{tilt}} \approx 1 \cdot U$  to  $E_{\text{tilt}} \approx 1.2 \cdot U$  for excitations near the phase transition, see e.g. Fig. 4. It is important to note that a similar effect was observed in experiments [7]. We found this shift present for all numbers of lattice sites we considered. The saturation times for lower order processes are of the order of  $1/J$ , i.e. the tunneling time (Fig. 5). The first order resonance saturates relatively quickly, after approximately one tunneling time. The higher order processes continue to increase in magnitude for a longer period: for the second order resonance at  $2 \cdot 1/J$ , saturation sets in at about  $2 \cdot 1/J$ . Third and fourth order processes take five tunneling times or longer to saturate.

With regard to the average number of atoms per well, we find that even in a small lattice such as ours, the qualitative features are not lost for non-commensurate filling factors. As shown in Fig. 6, while non-commensurate filling factors

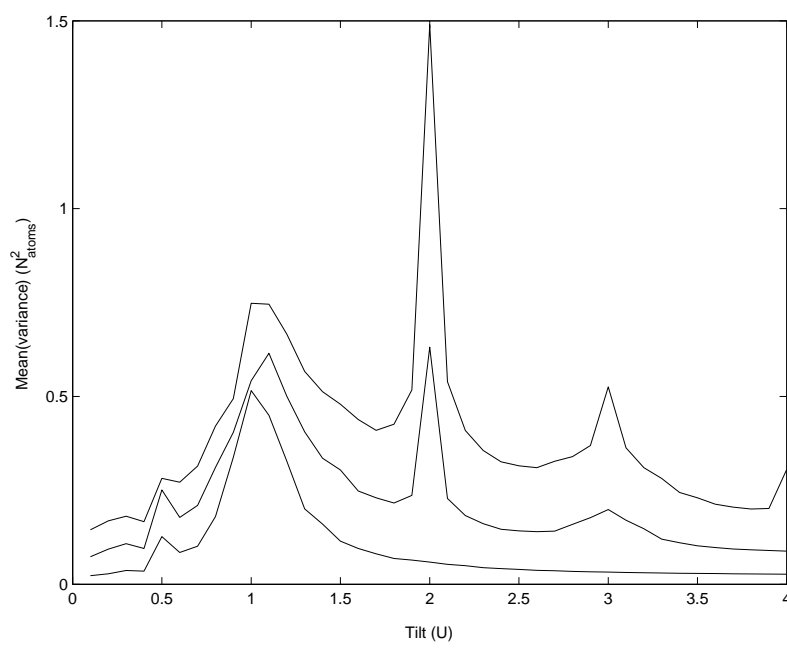


FIG. 3: Excitation pattern for  $\tau_{\text{perturb}} = 2/J$ ,  $U=20$ ,  $J=1$ , four lattice sites and  $n_{\text{av.occ.}} = 1, 2$  and  $3$  (bottom to top)

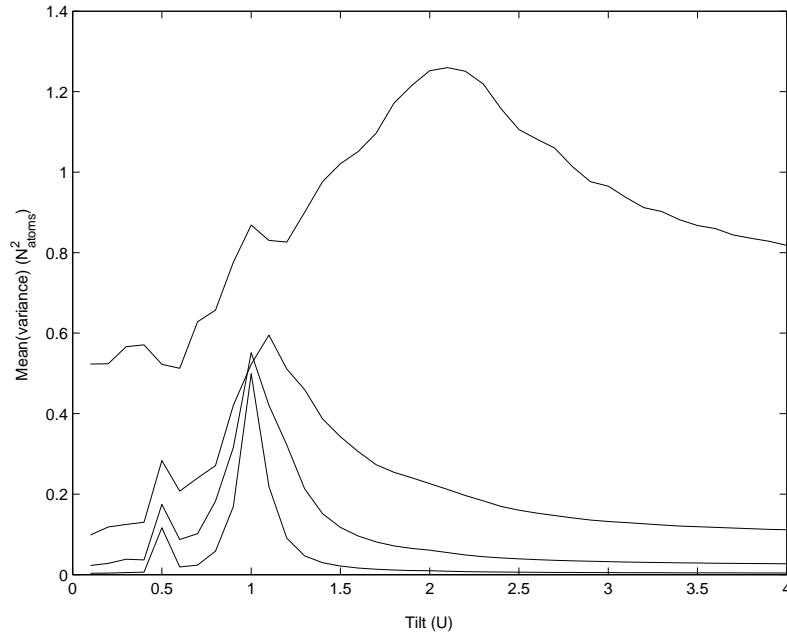


FIG. 4: This plot shows the dependence of excitations on initial squeezing. With increasing squeezing (plots are for  $U = 5, 10, 20$  and  $50$ ,  $J=1$  (constant), top to bottom, four lattice sites), resonance effects become noticeably narrower and the background decreases.

result in a more prominent continuous spectrum, they still show discrete Mott insulator peaks, albeit with somewhat greater widths. The background level is also significantly higher, as to be expected for defects. The actual excitations, however, are still clear.

We also compare results for different lattice sizes, ie for four to eight lattice sites. For more than five lattice sites and  $U/J \geq 20$ , the changes in results become very modest (see Fig. 7). Even for the smaller configurations, i.e. four and five sites, the important features are still in very good qualitative agreement. This leads us to be reasonably confident of the relevance of the principal features of our calculations for larger realistic systems.

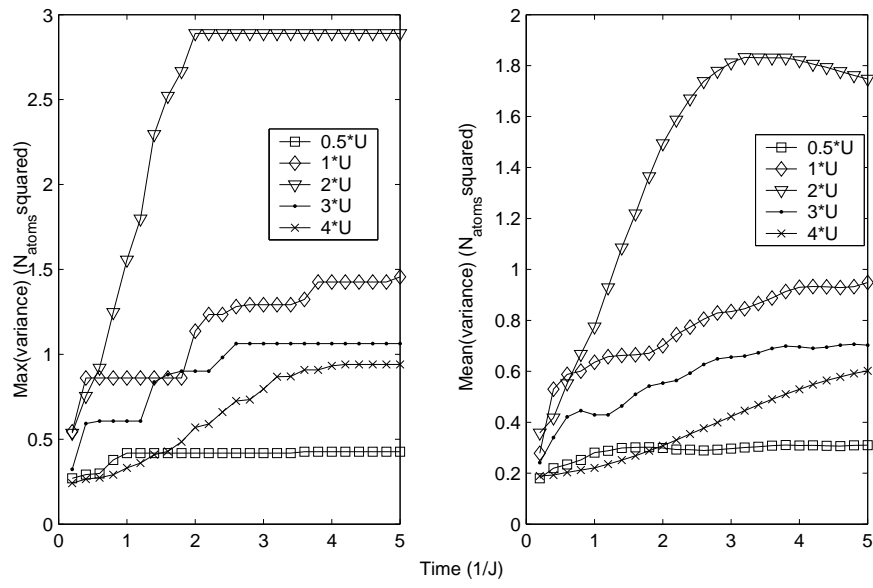


FIG. 5: This graph shows the changes in number variance for 0-5 perturbation times for the five most important peaks ( $0.5 \cdot U$ ,  $1 \cdot U$ ,  $2 \cdot U$ ,  $3 \cdot U$  and  $4 \cdot U$ ) and  $n_{av.occ.} = 3$ . The left plot shows the maximum value of the number variance, the right the average over the perturbation time.

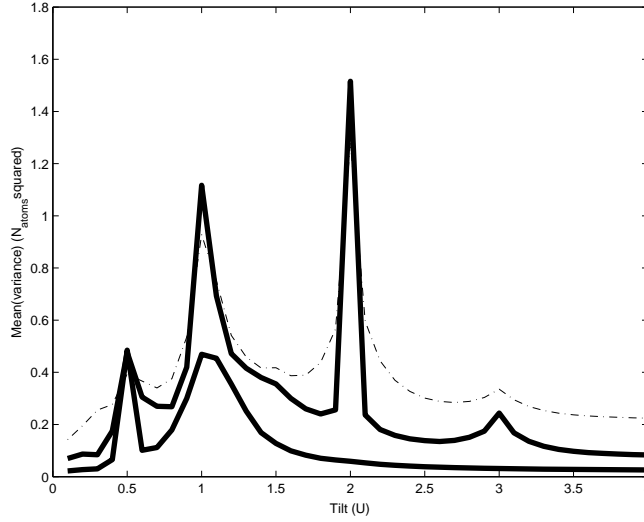


FIG. 6: The thick black lines are commensurate (upper  $n_{av.occ.} = 2$ , lower  $n_{av.occ.} = 1$ ), while the thin broken line shows results for  $n_{av.occ.} = 1.8$ . There are five lattice sites and  $U = 20$ ,  $J = 1$ .

#### IV. CONCLUSION

We have shown that the number variance is a indicator for the Mott insulator gap that is only weakly dependent on the size of the lattice. Using this diagnostic, we can confirm the origin of effects seen in recent experiments [4, 7]. In addition, we see higher order effects that fit very well into the simple picture of excitation of multiples of  $U$  in an infinite lattice. We find that the time dependency of the effects varies with the complexity of the underlying process: while the simplest nearest-neighbour hopping from one site to the next saturates in about a tunneling time, the higher order processes take longer. Our results indicate that even non-commensurate filling factors do not obscure the Mott insulator peaks in the number variance plots. This implies that they could be useful indicators even in non-ideal systems, such as lattices with defects.

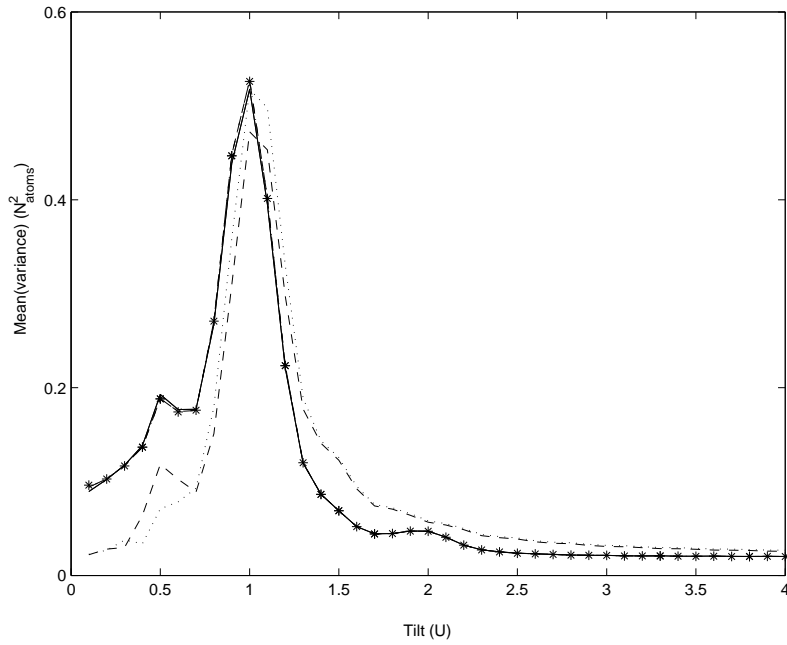


FIG. 7: Results for  $U = 20$ ,  $J = 1$  and  $\tau_{\text{perturb}} = 1/J$  for four to eight lattice sites. Dots: 4 wells, dashes line: 5 wells, solid line: 6 wells, dash-dot: 7 wells, stars: 8 wells

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